Boiling Point (Range)

201-15049B

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3

Robust Summary No.: OP E660

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the calculation method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential boiling point range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the boiling point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E660

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated BP (°C) / Measured* BP (°C) isopentane 30.18 27.8 toluene 125.72 110.6 m-xylene 148.29 139.1 styrene 146.65 145.0 naphthalene 231.64 217.9 tricyclodecane 171.25 na methylnaphthalene 249.60 241.1 * Experimental values from EPIWIN database. na = not available The data represent a potential boiling point range for substances represented by the 10 CAS numbers under Test Substance.
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E660

Conclusion:	The calculated boiling points for some representative constituents that are present in the category streams vary from 30.18 to 249.60°C @ 760 mm Hg. The measured boiling points of these same constituents vary from 27.8 to 241.1°C @ 760 mm Hg. Although this does not define the actual boiling points of the category streams, it offers an indication of a range that might be expected to encompass the boiling points of these complex streams with variable compositions. Boiling points outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 10 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E667

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery

	Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams: • **Pyrolysis C7s Fraction** • **Pyrolysis C7-C12 Fraction** • **Pyrolysis C7-C8 Fraction** • **C9+ From Xylene Unit** • **Hydrotreated C8-C10 Fraction** • **Hydrotreated C7-C12 Fraction** • **Hydrotreated C7+ Fraction** • **Hydrotreated C5/C9 blend** • **Toluene Extract** Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. **The Low Benzene Naphthas Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C12. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the nine process streams in this category are:

- **Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

    1. **Pyrolysis C7s Fraction** has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

    2. **Pyrolysis C7-C12 Fraction** has a typical composition including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics.

    3. **Pyrolysis C7-C8 Fraction** has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%.

- **C9+ from Xylene Unit** is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics.

- **Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend)** are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that

	will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions. 1. **Hydrotreated C8-C10 Fraction** has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range. 2. **Hydrotreated C7-C12 Fraction** is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins. 3. **Hydrotreated C7+ Fraction** is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins. 4. **Hydrotreated C5/C9 Blend** is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+. • **Toluene Extract** is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule. The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond.

The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Low Benzene Naphthas Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).

The substances in the Low Benzene Naphthas Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Low Benzene Naphthas Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.
3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.
4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3

Robust Summary No.: OP E667

Reliability:	These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo hydrolysis.
Reference:	American Chemistry Council, Olefins Panel. 2003. Hydrolysis Low Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E661

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. The Gold and Ogle Method is described by Lyman, W.J., 1985, In: Environmental Exposure from Chemicals. Volume 1. Neely, W.B. and Blau, G.E. (eds), Boca Raton, FL, CRC Press, Inc., Chapter 2.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential melting point range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the melting point range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E661

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated MP (°C) / Measured* MP (°C) isopentane -119.04 -159.9 toluene -59.17 -94.9 m-xylene -40.69 -47.8 styrene -48.31 -31.0 naphthalene 5.01 80.2 tricyclodecane -19.15 na methylnaphthalene 22.15 34.4 * Experimental values from EPIWIN database. na = not available The data represent a potential melting point range for substances represented by the 10 CAS numbers under Test Substance.
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E661

Conclusion:	The calculated melting points for some representative constituents that are present in the category streams vary from -119.04 to 22.15 °C. The measured melting points of these same constituents vary from -159.9 to 80.2°C. Although this does not define the actual melting points of the category streams, it offers an indication of a range that might be expected to encompass the melting points of these complex streams with variable compositions. Melting points outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the 10 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E663

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the log K_{ow} range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers listed under Test Substance. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E663

Results: (continued)

Units/Value:

Note: Deviations from protocol or guideline, analytical method.

Substance Constituent	Calculated log K_{ow} @ 25°C	Measured* log K_{ow} @ 25°C
isopentane	2.72	na
toluene	2.54	2.73
m-xylene	3.09	3.20
styrene	2.89	2.95
naphthalene	3.17	3.30
tricyclodecane	3.59	na
methylnaphthalene	3.72	3.86

* Experimental values from EPIWIN database.
na = not available
The data represent a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance.

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Partition Coefficient (Range)

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E663

Conclusion:	The calculated log K_{ow} for some representative constituents that are present in the category streams vary from 2.54 to 3.72 @ 25°C. The measured log K_{ow} of these same constituents vary from 2.73 to 3.86 @ 25°C. Although this does not define the actual log K_{ow} of the category streams, it offers an indication of a range that might be expected to encompass the log K_{ow} of these complex streams with variable compositions. Log K_{ow} values outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E668

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Low Benzene Naphthas Category. The Low Benzene Naphthas Category includes nine process streams: • **Pyrolysis C7s Fraction** • **Pyrolysis C7-C12 Fraction** • **Pyrolysis C7-C8 Fraction** • **C9+ From Xylene Unit** • **Hydrotreated C8-C10 Fraction** • **Hydrotreated C7-C12 Fraction** • **Hydrotreated C7+ Fraction** • **Hydrotreated C5/C9 blend** • **Toluene Extract**

Ten CAS numbers (see Test Substance) identify products derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis.

The Low Benzene Naphthas Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. This grouping of CAS numbers represents hydrocarbon streams with a carbon number distribution that is predominantly C5-C12. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low Benzene Naphthas.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the nine process streams in this category are:

- **Pyrolysis Fractions (C7s, C7-C12, and C7-C8 Fractions)** are separated by distillation into various boiling-point range fractions as intermediates in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

    1. **Pyrolysis C7s Fraction** has a carbon number distribution that is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

    2. **Pyrolysis C7-C12 Fraction** has a typical composition including about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene, with the balance expected to be largely unsaturated hydrocarbons and other aromatics.

3. **Pyrolysis C7-C8 Fraction** has a carbon number distribution that is predominantly C7 to C8. The reported compositions range from 45 to 80% with 11 to 78% C8 aromatics. The typical benzene concentration reported is 2% with a maximum of 5%.

- **C9+ from Xylene Unit** is a co-product from process units that produce o- or p-xylene. The carbon distribution for the stream is C8+ with some hydrocarbon compounds having a boiling point of 650°F or higher. The stream is predominantly aromatics.

- **Hydrotreated Pyrolysis Fractions (C8-C10, C7-C12, C7+ Fractions, and C5/C9 Blend)** are pyrolysis gasoline or distillate fractions of pyrolysis gasoline that are treated with hydrogen over catalyst. The hydrogenation process may be either one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert vinyl aromatics, for example, styrene to ethylbenzene. The second stage in a two-stage hydrogenation process is typically a vapor-phase, more severe hydrogenation that converts essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce high purity aromatics (toluene or xylenes in this case) is subjected to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from petroleum refineries are sometimes mixed with these pyrolysis fractions.

  1. **Hydrotreated C8-C10 Fraction** has a carbon number distribution of C6 to C12, but is predominantly C8 to C10. Typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.

  2. **Hydrotreated C7-C12 Fraction** is a distillate fraction of hydrogenated pygas with a carbon number distribution that is predominantly C7-C12, with lesser amounts of C6. Typical reported values indicate 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins.

  3. **Hydrotreated C7+ Fraction** is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream (alternately the stream could

be hydrotreated after distillation). The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. Typical reported values include 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.

4. **Hydrotreated C5/C9 Blend** is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Typical reported values includes approximately 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.

- **Toluene Extract** is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

Photolysis of Hydrocarbons

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2):

	<table><tr><th></th><th colspan="2">λ below 290 nm</th><th colspan="2">λ above 290 nm</th></tr><tr><th>Hydrocarbon</th><th>λ_{max}</th><th>ε</th><th>λ_{max}</th><th>ε</th></tr><tr><td>Ethylene</td><td>193</td><td>10,000</td><td>-</td><td>-</td></tr><tr><td>Benzene</td><td>255</td><td>215</td><td>-</td><td>-</td></tr><tr><td>Styrene</td><td>244 282</td><td>12,000 450</td><td>-</td><td>-</td></tr><tr><td>Naphthalene</td><td>221 270</td><td>100,000 5,000</td><td>311</td><td>250</td></tr></table> Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Low Benzene Naphthas category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2). Products in the Low Benzene Naphthas Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable
Degradation Products:** • **Note: Identification, concentration**	Unknown

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3

Robust Summary No.: OP E668

Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the Low Benzene Naphthas Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2003. Photodegradation (Direct): Low Benzene Naphthas Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E670

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E670

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The Low Benzene Naphthas Category** Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C11. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low Benzene Naphthas. The seven chemicals selected to represent the atmospheric oxidation potential of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3

Robust Summary No.: OP E670

Indirect Photolysis: (cont'd)** **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Chemical / Calculated* half-life (hrs) / OH- Rate Constant (cm^3/molecule-sec) isopentane 31.8 $4.0\ E^{-12}$ toluene 24.6 $5.2\ E^{-12}$ m-xylene 9.5 $13.6\ E^{-12}$ styrene 4.6 $28.1\ E^{-12}$ naphthalene 5.9 $21.6\ E^{-12}$ tricyclodecane 5.6 $22.9\ E^{-12}$ methylnaphthalene 2.3 $56.5\ E^{-12}$ * Atmospheric half-life values are based on a 12-hr day. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001). References: 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products:** • **Note: Identification, concentration**	Unknown

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E670

Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 2.3 to 31.8 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

** In IUCLID, provide additional discussion if needed in the results freetext

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E669

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E669

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

Calculated partitioning data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential distribution for substances represented by the 10 CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition.

Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the environmental distribution range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution			
Chemical	Air	Water	Soil	Sediment
isopentane	99.98	0.01	0.01	-
toluene	98.17	1.40	0.43	-
m-xylene	97.19	1.33	1.45	0.03
styrene	95.55	2.61	1.80	0.04
naphthalene	24.47	32.28	42.28	0.94
tricyclodecane	98.68	0.29	1.01	0.02
methylnaphthalene	97.68	0.40	1.88	0.04

* Distribution values determined using calculated input data from EPIWIN program

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E669

Results: (cont'd)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

	Measured** Percent Distribution			
Chemical	Air	Water	Soil	Sediment
Isopentane	99.98	0.01	0.01	-
toluene	98.80	0.81	0.39	-
m-xylene	97.91	0.86	1.20	0.03
styrene	96.65	1.85	1.46	0.04
naphthalene	42.27	20.56	36.33	0.81
tricyclodecane	na	na	na	na
methylnaphthalene	98.53	0.19	1.25	0.03

** Distribution values determined using measured input data from the EPIWIN program experimental database.
na = not available

Test Substance:

The Low Benzene Naphthas Category includes the following CAS numbers:

64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam-cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent.

More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E669

Conclusion:	The partitioning data represent a potential distribution range for substances in the 10 CAS numbers listed under Test Substance. Substances in the Low Benzene Naphthas Category are calculated to partition primarily to air with a negligible percentage partitioning to water, soil, and sediment. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the 10 CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E662

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the vapor pressure range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
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Results (continued): **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated VP (hPa @ 25°C) / Measured* VP (hPa @ 25°C) isopentane: 9.17 E2 / 9.19 E2 toluene: 31.60 / 37.86 m-xylene: 8.83 / 11.05 styrene: 6.73 / 8.53 naphthalene: 0.11 / 0.05 tricyclodecane: 2.64 / na methylnaphthalene: 4.60 E-2 / 7.33 E-2 * Experimental values from EPIWIN database. na = not available The data represent a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance.
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

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Robust Summary No.: OP E662

Conclusion:	The calculated vapor pressures for some representative constituents that are present in the category streams vary from 4.60 E-2 to 9.17 E2 hPa @ 25°C. The measured vapor pressures of these same constituents vary from 7.33 E-2 to 9.19 E2 hPa @ 25°C. Although this does not define the actual vapor pressures of the category streams, it offers an indication of a range that might be expected to encompass the vapor pressures of these complex streams with variable compositions. Vapor pressure outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

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Robust Summary No.: OP E664

LOW BENZENE NAPHTHAS ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the Low Benzene Naphthas Category are listed below. The data identify a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges for substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial substances in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly C5-C12. The seven chemicals selected to represent the water solubility range of this category are C5-C11 hydrocarbons that can be found in substances identified by the 10 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 64741-98-6; 64742-48-9; 64742-49-0; 64742-83-2; 68333-88-0; 68476-45-9; 68478-10-4; 68516-20-1; 68527-23-1; 68919-15-3
Robust Summary No.: OP E664

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) isopentane 184.6 na toluene 832.7 573.1 m-xylene 258.4 207.2 styrene 386.7 343.7 naphthalene 183.8 142.1 tricyclodecane 21.5 na methylnaphthalene 54.6 41.4 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance.
Test Substance:	The Low Benzene Naphthas Category includes the following CAS numbers: 64741-98-6 Extract, petroleum, heavy naphtha solvent 64742-48-9 Naphtha, petroleum, hydrotreated heavy 64742-49-0 Naphtha, petroleum, hydrotreated light 64742-83-2 Naphtha, petroleum, light steam-cracked 68333-88-0 Aromatic hydrocarbons, C9-C17 68476-45-9 Hydrocarbons, C5-10 aromatic concentration, ethylene-manufacture-by-product 68478-10-4 Naphtha, petroleum, light steam-cracked, debezenized, C8-16-cycloalkadiene concentrate 68516-20-1 Naphtha, petroleum, steam-cracked middle aromatic 68527-23-1 Naphtha, petroleum, light steam-cracked aromatic 68919-15-3 Hydrocarbons, C6-12, benzene-recovery Low Benzene Naphthas Category substances arise from production processes associated with ethylene manufacturing. The 10 CAS numbers are used to describe the nine process streams arising from the ethylene process and other associated manufacturing processes. The category includes hydrocarbon product streams associated with the ethylene industry. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. More information on the Low Benzene Naphthas Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low Benzene Naphthas Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

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Robust Summary No.: OP E664

Conclusion:	The calculated water solubility for some representative constituents that are present in the category streams vary from 21.5 to 832.7 mg/L @ 25°C. The measured water solubility of these same constituents vary from 41.4 to 573.1 mg/L @ 25°C. Although this does not define the actual water solubility of the category streams, it offers an indication of a range that might be expected to encompass the water solubility of these complex streams with variable compositions. Water solubilities outside these ranges may be possible for some category streams.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the 10 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low Benzene Naphthas Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 7/03)

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